Delocalization energy and bond multiplicity of graphite.

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Taking into account the bond multiplicity of graphite, one can simply calculate the delocalization energy of graphite.

The bond multiplicity of graphite is 1.54. To be precise, 1.538. This follows from the length of the C - C bond within one layer - 1.42 Å, from here we calculate the bond multiplicity (1.538) using the formula [1].

$$c-\text{c bond multiplicity} = -0.06040343 - \frac{5.67787529}{L} + \frac{11.28562201}{L^2}$$

$$\text{E of c}-\text{c bonds} = -2221.34518418 + \frac{5065.62912191}{L} - \frac{1699.18638789}{L^2}$$

c–c graphite multiplicity (L = 1.42 Å) = 1.538 ≈ 1.54

c–c benzene multiplicity (L = 1.397 Å) = 1.658

Ec–c graphite (L = 1.42 Å) = 503.3161 kj/mole

Ec–c benzene (L = 1.397 Å) = 534.0723 kj/mole

This means that both the aromaticity and the delocalization energy of graphite will be small, since the multiplicity is slightly greater than 1.5.

If we take into account that the energy of the C - C bond with a multiplicity of 1.5 is 493.3097 kJ/mol, and the energy of the C - C bond in the graphite layer is 503.3161 kJ/mol [1], then we can calculate the delocalization energy of graphite based on 6 carbon atoms. We take into account 6 bonds in one cycle, plus 3 more complete bonds outside the cycle, which is obvious based on the formula of graphite with a three-electron bond [1, p. 29].

ΔE = 503.3161 kJ/mol - 493.3097 kJ/mol = 10.0064 kJ/mol

10.0064 kJ/mol is the energy per C - C bond. So, for 6 carbon atoms we get a delocalization energy of 90.0576 kJ/mol.

ΔE = 9 * 10.0064 kJ/mol = 90.0576 kJ/mol (21.524 kcal/mol).

That is, graphite has a delocalization energy of 21.524 kcal/mol.

This is a small delocalization energy, but more than expected. Compare, benzene has a delocalization energy of 58.416 kcal/mol. That is, more than 2.7 times more. Considering the small bond multiplicity (1.54), the

delocalization energy of graphite is quite high. But if we recall the properties of graphite, then everything is in order.

At the end, I will add that there is a very weak interaction between the graphite layers, since the distance between the layers is 3.35 Å. Therefore, it is impossible to depict this interaction using classical formulas. In essence, this is already almost an intermolecular interaction, and it is for this reason that the graphite rod writes - the layers easily peel off.

1. Bezverkhniy V. D. Structure of the Benzene Molecule on the Basis of the Three-Electron Bond. SSRN Electronic Journal, Nov 2017. P. 10 - 11. https://dx.doi.org/10.2139/ssrn.3065241